

AD-A137 919

COMPUTATION OF CURRENT-VOLTAGE-CHARACTERISTICS IN A  
SEMICONDUCTOR DEVICE. (U) WISCONSIN UNIV-MADISON  
MATHEMATICS RESEARCH CENTER P A MARKOWICH ET AL.

1/1

UNCLASSIFIED

DEC 83 MRC-TSR-2605 DRAG29-80-C-0041

F/G 12/1

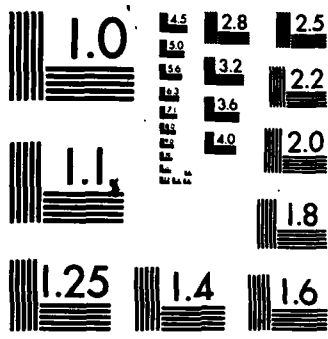
NL

END

FILED

3

DEC



MICROCOPY RESOLUTION TEST CHART  
NATIONAL BUREAU OF STANDARDS-1963-A

3

MRC Technical Summary Report #2605

COMPUTATION OF CURRENT-VOLTAGE-  
CHARACTERISTICS IN A SEMICONDUCTOR  
DEVICE USING ARC-LENGTH CONTINUATION

Peter A. Markowich, Christian A. Ringhofer,  
and Alois Steindl

AD A137919

Mathematics Research Center  
University of Wisconsin—Madison  
610 Walnut Street  
Madison, Wisconsin 53705

December 1983

(Received September 9, 1983)

DTIC  
ELECTE  
FEB 16 1984  
S B D

Approved for public release  
Distribution unlimited

Sponsored by

U. S. Army Research Office  
P. O. Box 12211  
Research Triangle Park  
North Carolina 27709

DTIC FILE COPY

84 02 15 160

UNIVERSITY OF WISCONSIN-MADISON  
MATHEMATICS RESEARCH CENTER

COMPUTATION OF CURRENT-VOLTAGE-CHARACTERISTICS IN A SEMICONDUCTOR  
DEVICE USING ARC-LENGTH CONTINUATION

Peter A. Markowich<sup>\*,1</sup>, Christian A. Ringhofer<sup>1</sup>, and Alois Steindl<sup>\*</sup>

Technical Summary Report #2605  
December 1983

ABSTRACT

This paper is concerned with the computation of semiconductor device current-voltage characteristics. We describe an algorithm which allows the computation of characteristics by continuation in a parameter which approximates the arclength of the characteristic. The use of this parameterization allows the characteristic to continue beyond snap-back-voltages, while continuation in the voltage fails past snap-back-voltages. We discuss the implementation of the parameterization and give a numerical example.

AMS (MOS) Subject Classifications: 35B30, 35P30

Key Words: Semiconductor devices, Characteristics, Continuation, Newton's method

Work Unit Number 3 (Numerical Analysis and Scientific Computing)

---

<sup>\*</sup>Institut für Angewandte und Numerische Mathematik, Technische Universität Wien, A-1040 Wien, Austria.

<sup>1</sup>Sponsored by the United States Army under Contract No. DAAG29-80-C-0041.

SIGNIFICANCE AND EXPLANATION

In this paper we present an algorithm for the numerical computation of current-voltage-characteristics in a semiconductor device (i.e. curves describing the dependence of the output current on the input voltage at some contacts). For certain devices (e.g. thyristors) the set of equations describing the state of the semiconductor device have multiple solutions for specific voltage ranges and snap-back phenomena occur (i.e. the current is not a single valued function of the voltage). This implies that the characteristic cannot be computed numerically by merely stepping up the voltage. <sup>The</sup> Our algorithm involves reparameterizing the characteristic curve by means of a parameter which approximates the arclength of the curve. Continuation in this parameter past snap-back-points does not cause serious difficulty.

<sup>The authors</sup>  
~~We~~ discuss the implementation of the reparameterization and present a numerical example.

Accession For	
NTIS	GRA&I <input checked="checked" type="checkbox"/>
DTIC	TAB <input type="checkbox"/>
Unannounced <input type="checkbox"/>	
Justification	
By	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A-1	



The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

# COMPUTATION OF CURRENT-VOLTAGE-CHARACTERISTICS IN A SEMICONDUCTOR DEVICE

## USING ARC-LENGTH CONTINUATION

Peter A. Markowich<sup>\*,1</sup>, Christian A. Ringhofer<sup>1</sup>, and Alois Steindl<sup>\*</sup>

### 1. Introduction

The computation of static current-voltage characteristics for devices which exhibit snap-back phenomena (like thyristors or even a pn-junction in the avalanche case) has created problems since continuation in the voltage does not work beyond snap-voltages. Figure 1 shows a typical characteristic of a thyristor in forward bias with the snap-back voltages  $U_{S1}$  and  $U_{S2}$ .

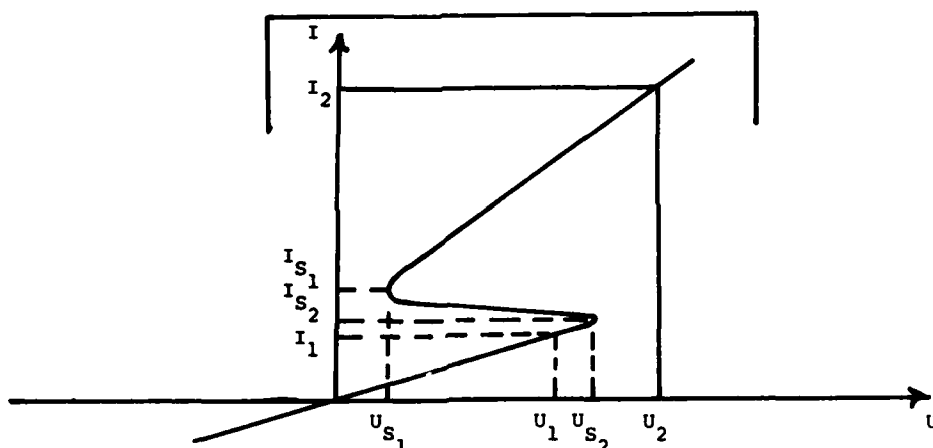


Figure 1. Current Voltage Characteristic of a Thyristor.

<sup>\*</sup>Institut für Angewandte und Numerische Mathematik, Technische Universität Wien, A-1040 Wien, Austria.

<sup>1</sup>Sponsored by the United States Army under Contract No. DAAG29-80-C-0041.

Assume that the point  $(U_1, I_1)$  was computed (say by starting at  $(0,0)$  and by gradually stepping up the voltage by the increment  $\Delta U$ ). Then, if  $U_2 = U_1 + \Delta U > U_{S_2}$ , the point  $(U_2, I_2)$  already lies on the upper branch of the characteristic and Newton's method for the numerical computation of  $(U_2, I_2)$  will probably fail when providing an initial guess which is computed just by using the previously computed solutions. The (dynamically stable) upper branch emerging from  $(U_{S_1}, I_{S_1})$  cannot be computed by continuation in  $U$  starting from some point on the (also dynamically stable) 'lower branch' connecting  $(0,0)$  and  $(U_{S_2}, I_{S_2})$ .

In this paper we demonstrate how to avoid this problem by introducing an arclength-type parameter. The characteristic can be computed past snap-back voltages when doing continuation in this new parameter. This procedure is well known to mathematicians, however, most semiconductor-device simulation codes do not make use of it yet.

We also demonstrate how an already existing code, which solves the fundamental semiconductor device equations for given contact voltages has to be augmented to accommodate the reparameterization. The augmentation turns out to be very cheap in programming as well as in computer resources.

Finally we present numerical results for a one-dimensional pn-junction in the avalanche case.

## 2. Statement of the Problem

The basic static semiconductor device equations as given by Van Roosbroeck (1950) are

$$\left. \begin{aligned} (2.1) \quad & \operatorname{div}(\epsilon \nabla \psi) = n - p - C \\ (2.2) \quad & \operatorname{div}(D_n \nabla n - \mu_n n \nabla \psi) = R \\ (2.3) \quad & \operatorname{div}(D_p \nabla p + \mu_p p \nabla \psi) = R \end{aligned} \right\} \quad x \in \Omega \subset \mathbb{R}^n, \quad n = 1, 2 \text{ or } 3.$$

(We employ the usual notation) where  $\Omega$  represents the device geometry. The electron and hole current densities are given by

$$(2.4) \quad J_n = q(D_n \nabla n - \mu_n n \nabla \psi),$$

$$(2.5) \quad J_p = -q(D_p \nabla p + \mu_p p \nabla \psi)$$

and the total current density

$$(2.6) \quad J = J_n + J_p.$$

For an MOS-device Laplace's equation

$$(2.7) \quad \operatorname{div}(\epsilon \nabla \psi) = 0, \quad x \in \phi$$

holds where  $\phi$  represents the oxide. The potential and the electrical displacement are assumed to be continuous at the interface  $\partial\Omega_{0g} = \partial\Omega \cap \partial\phi$  and electrons and holes are not allowed to penetrate the oxide ( $n$  and  $p$  vanish in  $\phi$ ). We assume that the device has  $r$  contacts  $C_1, \dots, C_r$ . At these contacts the boundary conditions

$$(2.8) \quad \psi|_{C_i} = \tilde{\psi} + U_i$$

are prescribed where  $\tilde{\psi}$  denotes the built in potential at the contact if  $C_i$  is Ohmic, the negative flat-band voltage if  $C_i$  is a gate contact on the metal-semiconductor interface. Mark function if  $C_i$  is a Schottky contact.  $U_i$  is the potential applied to  $C_i$ .

Also  $n$  and  $p$  are prescribed at Ohmic and Schottky contacts.

The remaining part of the boundary of the device is assumed to be insulating, that means the derivatives of  $\psi$ ,  $n$  and  $p$  in normal direction to the boundary vanish there.



The outflow current density of  $C_2$  is given by

$$(2.9) \quad I_2 = \int_{C_2} \mathbf{J} \cdot \mathbf{n} ds,$$

where  $\mathbf{n}$  denotes the exterior unit normal vector to  $C_1$ .

For the following we write the problem (2.1)-(2.3) (and (2.7) for a MOS device) subject to the mentioned boundary conditions (and interface condition for a MOS device) or a scaled version of it in operator form:

$$(2.10) \quad A(z, U_1, \dots, U_r) = 0, \quad z = (\psi, n, p)$$

while

$$(2.11) \quad A : Z \times \mathbb{R}^r \rightarrow Y$$

where  $Z$  and  $Y$  are appropriate (Banach) spaces of functions. In the sequel we are interested in the determination of the outflow current  $I_1$  for varying contact voltage  $U_j \in \mathbb{R}$  and fixed voltages  $U_1, \dots, U_{j-1}, U_{j+1}, \dots, U_r$ . For notational simplicity we set  $U := U_1$ ,  $I := I_1$ . We assume that the resulting current-voltage (I-U)-characteristic is a smooth curve in  $\mathbb{R}^2$  which can be parameterized as follows

$$(2.12) \quad U = U(s), \quad I = I(s)$$

where

$$(2.13) \quad \dot{U}^2(s) + \dot{I}^2(s) = 1 \quad (\cdot \text{ denotes } \frac{d}{ds}).$$

Then  $s - s_0$  is the length of the arc connecting  $(U(s_0), I(s_0))$  and  $(U(s), I(s))$ .

The goal of the analysis following this section is to facilitate the numerical computation of the curve (2.12). For further notational simplicity we denote

$$(2.14) \quad B(z, U) = A(z, U_1, \dots, U_{j-1}, U, U_{j+1}, \dots, U_r)$$

(all contact voltages except  $U_j = U$  are fixed) where

$$(2.15) \quad B : Z \times \mathbb{R} \rightarrow Y.$$

### 3. Parameterization

The arclength parameterization (2.13) is not suited for computational purposes and therefore we use the approximation

$$(3.1) \quad \dot{I}(\tau_0)(I - I(\tau_0)) + \dot{U}(\tau_0)(U - U(\tau_0)) - (\tau - \tau_0) = 0$$

for  $\tau$  sufficiently close to  $\tau_0$  assuming that  $(U_0, I_0) := (U(\tau_0), I(\tau_0))$  and the unit tangent-vector  $(\dot{U}_0, \dot{I}_0) := (\dot{U}(\tau_0), \dot{I}(\tau_0))$  are known.

Noting that  $I$  as given by (2.9) (for  $l = i$ ) is a functional of  $z$ , i.e.

$I = I[z]$  we denote (3.1) by

$$(3.2) \quad N(z, U, \tau) = 0, \quad N : Z \times \mathbb{R}^2 \rightarrow \mathbb{R}$$

and augment  $B(z, U) = 0$  by (3.2), that means we solve

$$(3.3) \quad P(y, \tau) = \begin{pmatrix} B(y) \\ N(y, \tau) \end{pmatrix} = 0, \quad y = (z, U)$$

where  $\tau$  is in a sufficiently small neighborhood of  $\tau_0$ . We will show that the I-U-characteristic can be computed by solving (3.3) by continuation in  $\tau$  (at least locally about  $\tau_0$ ) even if  $U_0$  is a snap-back voltage.

A geometrical algorithm for the determination of  $(U(\tau), I(\tau))$  as defined by (3.1) is as follows. At first the point  $S_0$  on the tangent to  $(U_0, I_0)$ , whose distance to  $(U_0, I_0)$  is  $|\tau - \tau_0|$  (if  $\tau - \tau_0 > 0$  the vector pointing from  $(U_0, I_0)$  to  $S_0$  is oriented as the tangent vector  $(\dot{U}_0, \dot{I}_0)$  and if  $\tau - \tau_0 < 0$  it is oriented in the opposite direction) is determined. The normal to the tangent through  $S_0$  is intersected with the characteristic curve giving  $(U(\tau), I(\tau))$ . This is illustrated in Figure 2 at a 'regular point' (a non-snap-back-point) of the characteristic.

Figure 3 demonstrates the reparameterization at a snap-back-point  $(U_0, I_0)$ . It is intuitively clear that  $(U(\tau), I(\tau))$  can be determined in a locally unique way if  $|\tau - \tau_0|$  is sufficiently small.

To prove this we define 'regular points' and 'simple limit points' (i.e. snap-back points) mathematically (see H. Keller (1977)).

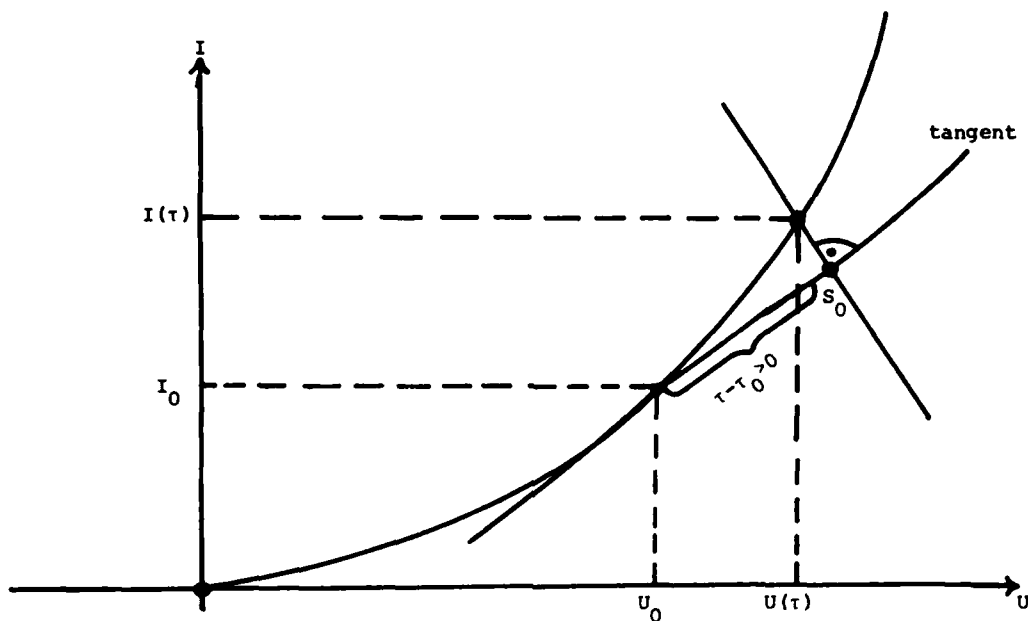


Figure 2. A Regular Point

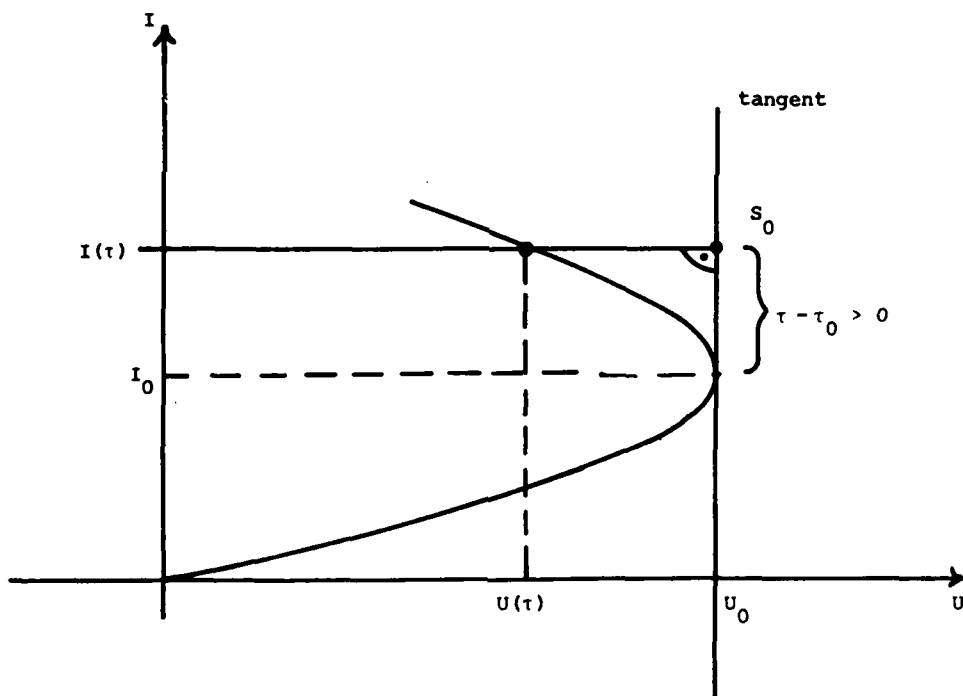


Figure 3. A 'Snap-back Point'

For the reader who is not familiar with the concepts of nonlinear analysis in Banach spaces we remark that, for understanding the implications of the following, it suffices to regard  $B$  as a function from  $\mathbb{R}^{K+1}$  into  $\mathbb{R}^K$  and  $N$  as a function from  $\mathbb{R}^{K+2}$  into  $\mathbb{R}$  for some integer  $K$ . Then Frechet derivatives (linearizations) are then Jacobi matrices of corresponding dimensions. This corresponds to analyzing an appropriate discretization of the semiconductor device equations (subject to the mentioned boundary conditions) and of (3.1).

We define:

- 1) The point  $(z_0, U_0)$  ( $z_0 := z(s_0)$ ) is the solution of  $B(z, U_0) = 0$  with  $I_0 = I[z_0]$  is called regular solution point of  $B(z, U) = 0$  if the Frechet derivative  $\frac{\partial B}{\partial z}(z_0, U_0)$  is one-to-one and onto (i.e. invertible).
- 2) The point  $(z_0, U_0)$  is called normal limit solution point of  $B(z, U) = 0$  if  $N(\frac{\partial B}{\partial z}(z_0, U_0))$  is one dimensional ( $N(A)$  denotes the null space of the operator  $A$ ), the codimension of  $R(\frac{\partial B}{\partial z}(z_0, U_0))$  is one ( $R(A)$  denotes the range of the operator  $A$ ) and if  $\frac{\partial B}{\partial U}(z_0, U_0) \notin R(\frac{\partial B}{\partial z}(z_0, U_0))$ .

The following Theorem is along the lines of Keller's (1977) Theorem 3.3.

**Theorem 3.1:** Let  $(z_0, U_0)$  be either a regular solution or a normal limit solution of  $B(z, U) = 0$ . If  $B$  is sufficiently smooth then for  $(\tau - \tau_0)$  sufficiently small there exists a unique smooth arc of solutions  $(z(\tau), U(\tau))$  of  $B(z, U) = 0$  passing through  $(z_0, U_0)$  and fulfilling (3.3). The Frechet derivatives  $\frac{\partial P}{\partial(z, U)}$  are one-to-one and onto along this arc.

Proof:

$$C_0 := \frac{\partial P}{\partial(z, U)}(z_0, U_0, \tau_0) = \begin{pmatrix} \frac{\partial B}{\partial z}(z_0, U_0) & \frac{\partial B}{\partial U}(z_0, U_0) \\ \dot{I}(\tau_0) \frac{\partial I}{\partial z}[z_0] & \dot{U}(\tau_0) \end{pmatrix}$$

holds. If  $(z_0, U_0)$  is a regular solution point of  $B(z, U) = 0$ , then  $\frac{\partial B}{\partial z}(z_0, U_0)$  is one-to-one and onto. To show that  $\frac{\partial P}{\partial(z, U)}(z_0, U_0, \tau_0)$  is one-to-one and onto it suffices to prove that

$$(3.4) \quad \alpha_0 := \dot{U}(\tau_0) - \dot{I}(\tau_0) \frac{\partial I}{\partial z} [z_0] \left( \frac{\partial B}{\partial z} (z_0, U_0) \right)^{-1} \frac{\partial B}{\partial U} (z_0, U_0) \neq 0$$

holds (see Keller (1977), Lemma 2.8)). By differentiating  $B(z, U) = 0$  with respect to  $S$  we obtain at  $S = \tau_0$

$$(3.5) \quad \frac{\partial B}{\partial z} (z_0, U_0) \dot{z}(\tau_0) + \frac{\partial B}{\partial U} (z_0, U_0) \dot{U}(\tau_0) = 0.$$

$\dot{U}(\tau_0) = 0$  implies  $\dot{z}(\tau_0) = 0$  (because of the nonsingularity of  $\frac{\partial B}{\partial z} (z_0, U_0)$ ) and  $\dot{I}(\tau_0) = \frac{\partial I}{\partial z} [z_0] \dot{z}(\tau_0) = 0$  follows which contradicts (2.13). Therefore  $\dot{U}(\tau_0) \neq 0$  and

$$\left( \frac{\partial B}{\partial z} (z_0, U_0) \right)^{-1} \frac{\partial B}{\partial U} (z_0, U_0) = - \frac{\dot{z}(\tau_0)}{\dot{U}(\tau_0)}$$

holds. Inserting this into (3.4) gives

$$\alpha_0 = \dot{U}(\tau_0) + \dot{I}(\tau_0) \frac{\partial I}{\partial z} [z_0] \frac{\dot{z}(\tau_0)}{\dot{U}(\tau_0)}.$$

Thus

$$\alpha_0 \dot{U}(\tau_0) = \dot{U}^2(\tau_0) + \dot{I}^2(\tau_0) = 1 \Rightarrow \alpha_0 \neq 0$$

and  $C_0$  is one-to-one and onto.

Now let  $(z_0, U_0)$  be a normal limit solution of  $B(z, U) = 0$ , (3.5) implies

$$\frac{\partial B}{\partial z} (z_0, U_0) \dot{z}(\tau_0) = - \frac{\partial B}{\partial U} (z_0, U_0) \dot{U}(\tau_0) = 0$$

because  $\frac{\partial B}{\partial U} (z_0, U_0) \notin R(\frac{\partial B}{\partial z} (z_0, U_0))$ . Since  $\frac{\partial B}{\partial U} (z_0, U_0)$  is not the null-operator

$\dot{U}(\tau_0) = 0$  follows (compare to Figure 3). Therefore  $N(\frac{\partial B}{\partial z} (z_0, U_0)) = \text{span}\{\dot{z}(\tau_0)\}$  holds. Keller's (1977) Lemma 2.8 implies that  $C_0$  is one-to-one and onto iff

$$(3.6) \quad \dim R(\dot{I}(\tau_0) \frac{\partial I}{\partial z} [z_0]) = 1$$

$$(3.7) \quad \dot{I}(\tau_0) \frac{\partial I}{\partial z} [z_0] \notin N(\frac{\partial B}{\partial z} (z_0, U_0))$$

hold. Obviously

$$\dot{I}(\tau_0) \frac{\partial I}{\partial z} [z_0] \dot{z}_0 = \dot{I}^2(\tau_0) = 1$$

holds because of (2.13) ( $\dot{U}(\tau_0) = 0$ ) and (3.6), (3.7) follow.

The invertibility of  $C_0$  and the implicit function theorem (see Schwartz (1969)) imply Theorem 3.1.  $\square$

The Theorem implies that - at least for  $|\tau - \tau_0|$  sufficiently small - the solution arc of  $B(z,U) = 0$  can be computed by solving (3.3) (which is the 'reparameterized version of  $B(z,U) = 0$ ) for  $z$  and  $U$  (by continuation in  $\tau$ ) using Newton's method which is quadratically convergent along the whole solution arc.

#### 4. Implementation

For the numerical solution of the fundamental semiconductor device equations  $B(z, U) = 0$  the problem has to be discretized appropriately, that means  $B_h(z_h, U) = 0$  has to be solved instead of  $B(z, U) = 0$  ( $h$  represents the grid parameter). For a collection of results on discretization methods see Mock (1983).

We now assume that  $B_h$  has already been chosen and that  $B_h : \mathbb{R}^{K+1} \rightarrow \mathbb{R}^K$ . Also an appropriate numerical integration rule  $I_h[z_h]$  has to be used to discretize

$$I[z] = \int_{C_1} I \cdot nds.$$

To get the continuation started at  $S = S_0$  we solve  $B_h(z_h, U_0) = 0$  obtaining  $z_{h_0}$  (we assume that  $(z_{h_0}, U_0) =: (z_h(\tau_0), U(\tau_0))$  is a regular solution of  $B(z_h, U) = 0$ ) and  $(I_{h_0} := I_h[z_{h_0}])$ . An approximation of the tangent vector to the  $I - U$  characteristic at  $(U_0, I_0)$  can be obtained by solving  $B_h(z_h, \tilde{U}_0) = 0$  (with  $\Delta U_0 = \tilde{U}_0 - U_0$  suff. small) for  $z_h = \tilde{z}_{h_0}$  and by setting

$$\dot{U}_0 = \frac{\tilde{U}_0 - U_0}{\omega}, \quad \dot{I}_0 = \frac{I_h[\tilde{z}_{h_0}] - I_h[z_{h_0}]}{\omega}$$

$$\text{with } \omega = \sqrt{(\tilde{U}_0 - U_0)^2 + (I_h[\tilde{z}_{h_0}] - I_h[z_{h_0}])^2}.$$

Assume now that we already solved

$$(4.1) \quad N_h(z_h, U_h, \tau) \equiv \begin{pmatrix} B_h(z_h, U_h) \\ N(z_h, U_h, \tau) \end{pmatrix} = 0$$

for  $\tau = \tau_K$  (i.e.  $(z_h(\tau_K), U_h(\tau_K))$  and  $I_h(\tau_K)$  are known). We compute

$$(z'_h(\tau_K), U'_h(\tau_K)) := \left( \frac{d}{d\tau} z_h(\tau_K), \frac{d}{d\tau} U_h(\tau_K) \right) \text{ from}$$

$$(4.2) \quad \frac{d}{d\tau} N_h(z_h, U_h, \tau_K) = \begin{pmatrix} \frac{\partial B_h}{\partial z}(z_h(\tau_K), U_h(\tau_K)) & \frac{\partial B_h}{\partial U}(z_h(\tau_K), U_h(\tau_K)) \\ \dot{I}(\tau_0) \frac{\partial I_h}{\partial z_h}[z_h(\tau_K)] & \dot{U}(\tau_0) \end{pmatrix} \begin{pmatrix} \dot{z}_h(\tau_K) \\ \dot{U}(\tau_K) \end{pmatrix} + \begin{pmatrix} 0 \\ -1 \end{pmatrix} = 0$$

and obtain  $I'_h(\tau_K) = \frac{\partial I_h}{\partial z_h} [z_h(\tau_K)] z'_h(\tau_K)$ . For the continuation we choose  $\Delta\tau_K$ , set  $\tau_{K+1} = \tau_K + \Delta\tau_K$  and solve (4.1) for  $\tau = \tau_{K+1}$ . As initial guess for the iteration procedure for the numerical solution of (4.1) we pick the Euler predictor

$$(4.3) \quad \begin{pmatrix} z_h^{(0)}(\tau_{K+1}) \\ U_h^{(0)}(\tau_{K+1}) \end{pmatrix} = \begin{pmatrix} z_h(\tau_K) \\ U_h(\tau_K) \end{pmatrix} + \Delta\tau_K \begin{pmatrix} z'_h(\tau_K) \\ U'_h(\tau_K) \end{pmatrix}.$$

If the I-U-characteristic consists only of regular and limit points then it follows from Keller (1975) and from Theorem 3.1 (we assume that  $\tau_{K+1}$  is suff. close to  $\tau_0$  such that Theorem 3.1 holds for  $\tau = \tau_{K+1}$ ) that Newton's method converges quadratically if  $\Delta\tau_K$  is sufficiently small, and if  $P_h$  is a stable and consistent (see Keller (1975)) approximation to  $P$ .

Since Theorem 3.1 implies that  $\frac{\partial P}{\partial(z,U)}(z(\tau), U(\tau), \tau)$  is nonsingular if  $|\tau - \tau_0|$  is suff. small it is recommendable to update  $\tau_0$  (and  $N$ ) after a few continuation steps. This is done by setting:

$$(4.4)(a) \quad \tau_0^{(NEW)} := \tau_{L+1}$$

and

$$(4.4)(b) \quad (\dot{U}(\tau_0^{(NEW)}), \dot{I}(\tau_0^{(NEW)})) := \frac{(U'(\tau_{L+1}), I'(\tau_{L+1}))}{\sqrt{(U'(\tau_{L+1}))^2 + (I'(\tau_{L+1}))^2}}.$$

A way to determine when an update is desirable is to require that the length of the tangent vector  $(U'(\tau_K), I'(\tau_K))$  differs from 1 by less than a certain prescribed error tolerance.

Of course, the sign of the increments  $\Delta\tau_K$  has to be constant throughout the whole continuation process (and equal to the sign of  $\Delta U_0$ ). For the thyristor characteristic with  $U_0 = I_0 = 0$ ,  $\tau_0 = 0$  positive increments ( $\Delta U_0 > 0, \Delta\tau_K > 0$ ) imply that one 'walks up' the forward characteristic ( $U > 0$ ) and negative increments ( $\Delta U_0 < 0, \Delta\tau_K < 0$ ) result in the computation of the reverse characteristic ( $U < 0$ ).



The increments  $\Delta\tau_K$  have to be chosen such that the initial guess (4.3) lies in the domain of attraction of the iteration method for (4.1) at  $\tau = \tau_{K+1}$ . For a sufficiently smooth solution arc

$$(4.5) \quad \begin{pmatrix} z_h(\tau_{K+1}) \\ u_h(\tau_{K+1}) \end{pmatrix} - \begin{pmatrix} z_h^{(0)}(\tau_{K+1}) \\ u_h^{(0)}(\tau_{K+1}) \end{pmatrix} = \frac{(\Delta\tau_K)^2}{2} \begin{pmatrix} z_h''(\xi_K) \\ u_h''(\xi_K) \end{pmatrix}, \quad \xi_K \in (\tau_K, \tau_{K+1})$$

holds. Therefore one has to require that

$$(4.6) \quad |\Delta\tau_K| \lesssim [(2\|z_h''\|_{[\tau_K, \tau_{K+1}]} + 2\|u_h''\|_{[\tau_K, \tau_{K+1}]})\delta_{K+1}]^{\frac{1}{2}}$$

where  $\delta_{K+1}$  represents the convergence radius of the iterative method for the approximate solution of (4.1) at  $\tau = \tau_{K+1}$ . Computable estimates for  $\delta_{K+1}$  and strategies slightly different from (4.6) can be found in Den Heizer and Rheinboldt (1981).

Assume now that a Newton-type procedure is used as iteration-method. Then a linear system of the form

$$(4.7) \quad \begin{pmatrix} a_h & b_h \\ c_h & d \end{pmatrix} \begin{pmatrix} \delta z_h \\ \delta u_h \end{pmatrix} = \begin{pmatrix} v_h \\ w_h \end{pmatrix}$$

has to be solved at every iteration step (and also for solving (4.2)) with

$$(4.8) \quad \left. \begin{aligned} a_h &= \frac{\partial B_h}{\partial z_h} \\ b_h &= \frac{\partial B_h}{\partial U} \\ c_h &= \frac{\partial N_h}{\partial z_h} \\ d &= \frac{\partial N_h}{\partial U} \end{aligned} \right\} \begin{aligned} &\text{evaluated at some iterate} \\ &(z_h^{(l)}, u_h^{(l)}) \quad \text{and} \quad \tau = \tau_K. \end{aligned}$$

If a Gauss-solver for sparse matrices is used to solve systems of the form  $A_h z_h = r_h$  (which occur in solving the fundamental semiconductor device equations (2.10) for prescribed contact-voltages) then it can easily be modified to solve systems of the form (5.7). The  $K + 1$ -st row  $\begin{pmatrix} b_h \\ d \end{pmatrix}$  and the  $K + 1$ -st column  $(c_h, d)$  do not create additional fill-in during the elimination process.

If a band-solver is used to solve systems with coefficient matrices  $A_h$  then systems of the form (4.7) can be solved as suggested in Keller (1977), that is by solving two systems with coefficient matrix  $A_h$  simultaneously. This, of course, only gives accurate results when  $A_h$  has a moderate condition number, i.e. when  $r_K$  does not correspond to a limit point. However, it is possible to continue beyond limit points when using the parameterization (3.1) (see Keller (1977), Theorem 4.4).

### 5. A Test Problem

As a test problem we applied the arclength-continuation procedure to the one-dimensional semiconductor device equations modelling a silicon pn-junction in the avalanche case.

For simplicity we took an odd, piecewise continuous doping profile (see Figure 4).

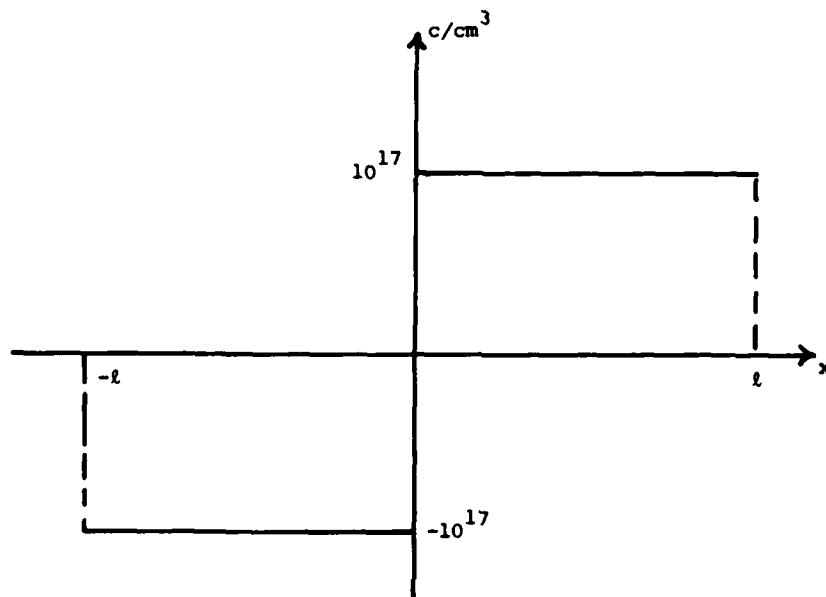


Figure 4. Doping Profile

The length of the pn-junction is  $2l = 5 \times 10^{-3} \text{cm}$ .

The avalanche phenomenon was modelled by the generation rate

$$(5.1) \quad R = -\alpha(\psi')(|J_n| + |J_p|)$$

with  $J_n, J_p$  given by (2.4), (2.5) resp. The following expression was used for the hole and electron ion isolation rate:

$$(5.2) \quad \alpha(\psi'(x)) = \sigma_1 \exp\left(-\frac{\sigma_2}{|\psi'(x)|}\right); \quad \sigma_1, \sigma_2 > 0.$$

The electron and hole mobilities were taken equal (also the electron and hole diffusivities). The obtained results should not be regarded as physically significant, they however illustrate very well the power of the reparameterization technique.

We remark that in the one-dimensional case the current is constant and given by

$$(5.3) \quad I \equiv q(D_n(n' - p') - \mu_n(n + p)\psi') \quad (\text{for } D_n = D_p, \mu_n = \mu_p) .$$

A scaled version of (2.1)-(2.3) (see Markowich (1983a) for the scaling) was discretized by using the three-point-scheme for Poisson's equation and the Scharfetter-Gummel scheme for the continuity equations (see Markowich *et al.* (1983)).

The functional  $I_h[z_h]$  was obtained by discretizing the current (5.3) at the largest grid point  $x_1$  with  $x_1 < 1$  also using the Scharfetter-Gummel discretization.

Figure 5 shows the obtained I-U-characteristic for  $-5U_T < U < 0$  ( $U_T$  is the thermal voltage). The onset of avalanche generation occurs at  $U = -1.5U_T$  and the current increases linearly (in absolute value) beyond that. This linear increase continues as far as  $U = -200U_T$ . Then the increase gets faster and the snap-back occurs at  $U = -240U_T$  (see Figure 6). The continuation of the solution arc beyond the limit point was no problem.

Figures 7 and 8 show  $\int_{-1}^1 \alpha(\psi'(s))ds$  over the applied bias. For  $U = 0$  (equilibrium solution)  $\int_{-1}^1 \alpha(\psi')ds < 1$ , then it increases until it equals 1. This happens around that U-value at which avalanche generation starts, i.e.  $U = -1.5U_T$  (compare to Figure 5). Then  $\int_{-1}^1 \alpha(\psi')ds$  remains almost constant until close to the snap-back voltage (see Figure 4). Slightly before the snap-back voltage it increases and gets significantly larger than 1. It was often claimed (see, for example, Sze (1981)) that 'breakdown' happens at that voltage at which  $\int_{-1}^1 \alpha(\psi')ds$  reaches one. This is not true in the mathematical sense for our simple model, there is a continuous branch of solutions (of the one-dimensional semiconductor problem in the case of avalanche generation) which emerges at the equilibrium solution (for  $U = 0$ ) and which contains at least one solution for every  $U < 0$  (see Markowich (1983b)). The situation, however, might change if temperature is introduced as unknown quantity.

# J-U-CHARACTERISTIC

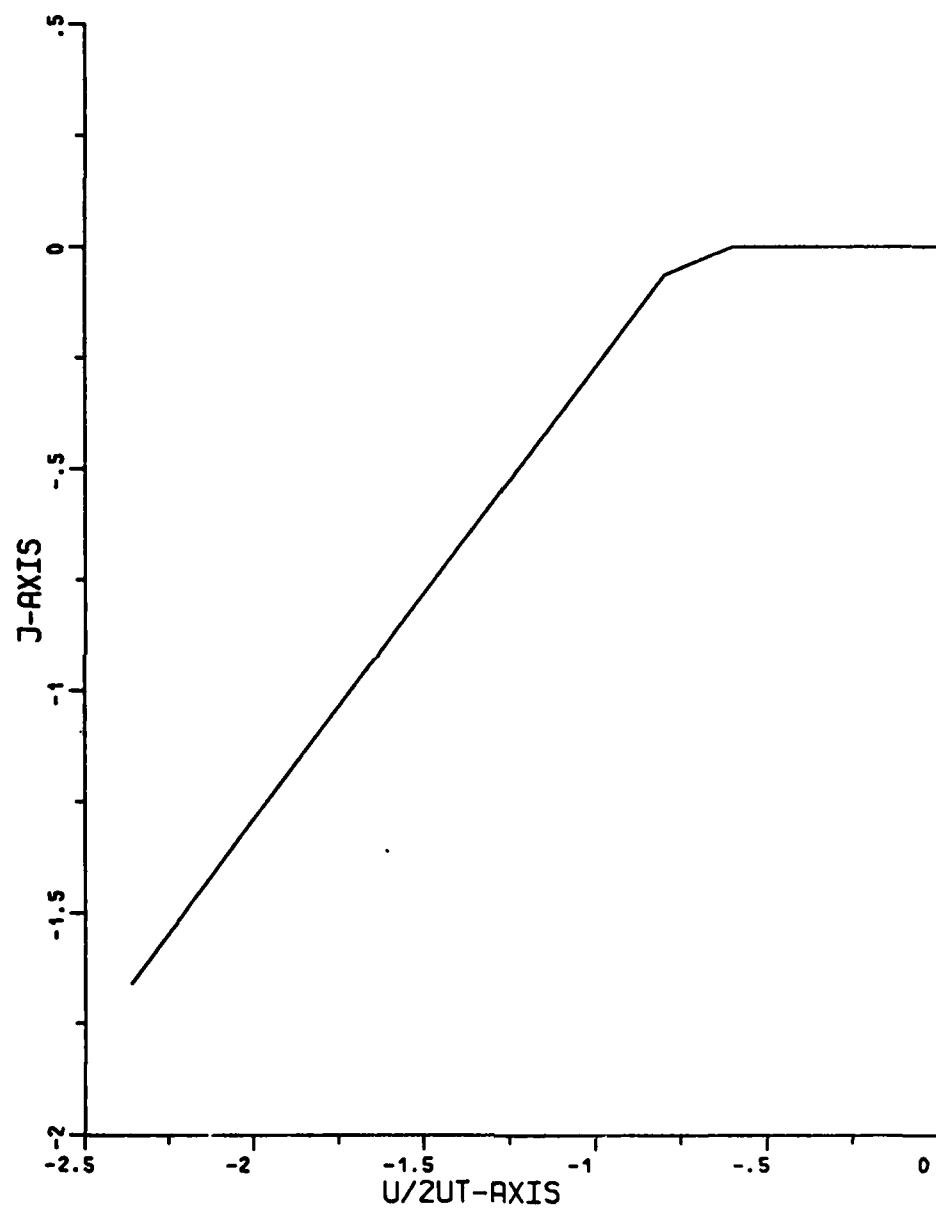


Figure 5

# J-U-CHARACTERISTIC

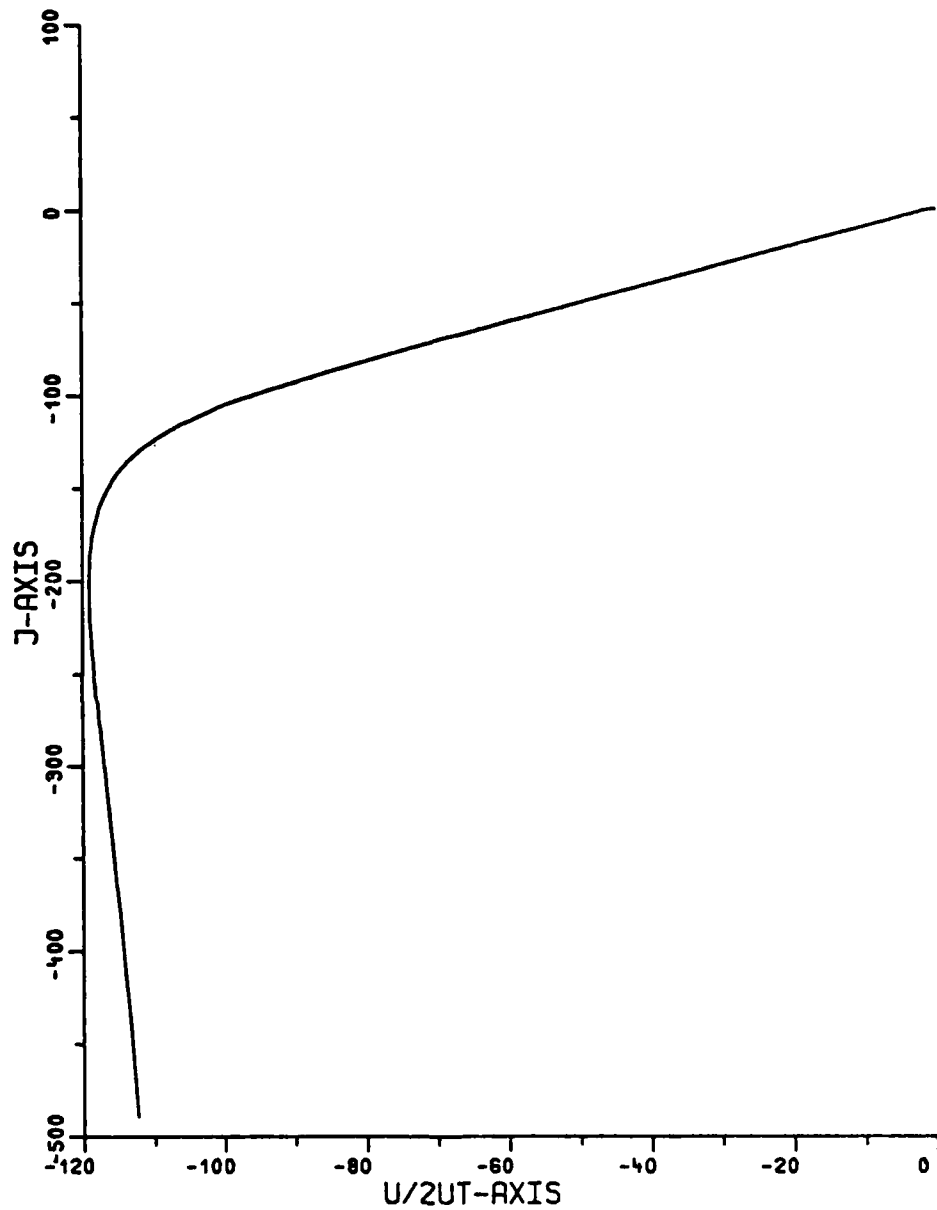


Figure 6

# INT (ALPHA) OVER APPLIED BIAS

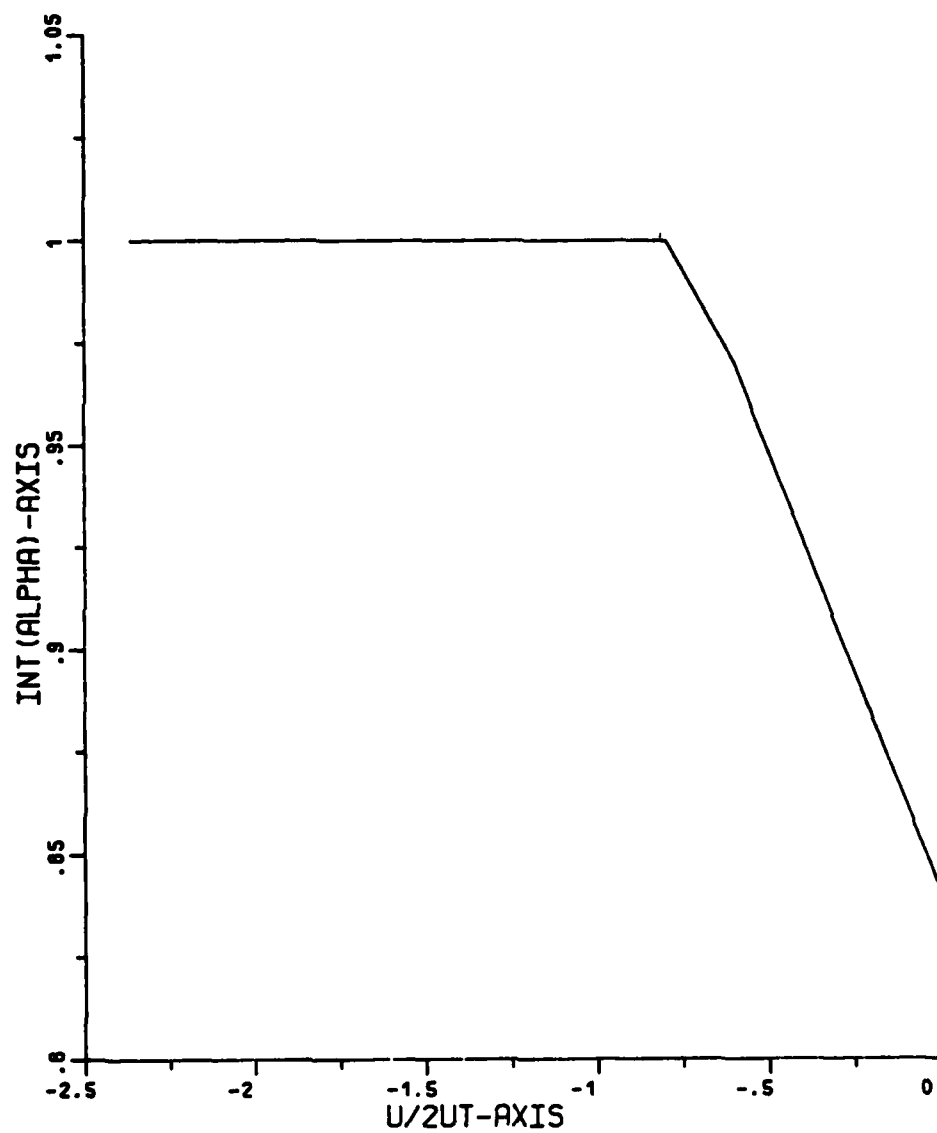


Figure 7

INT (ALPHA)  
OVER APPLIED BIAS

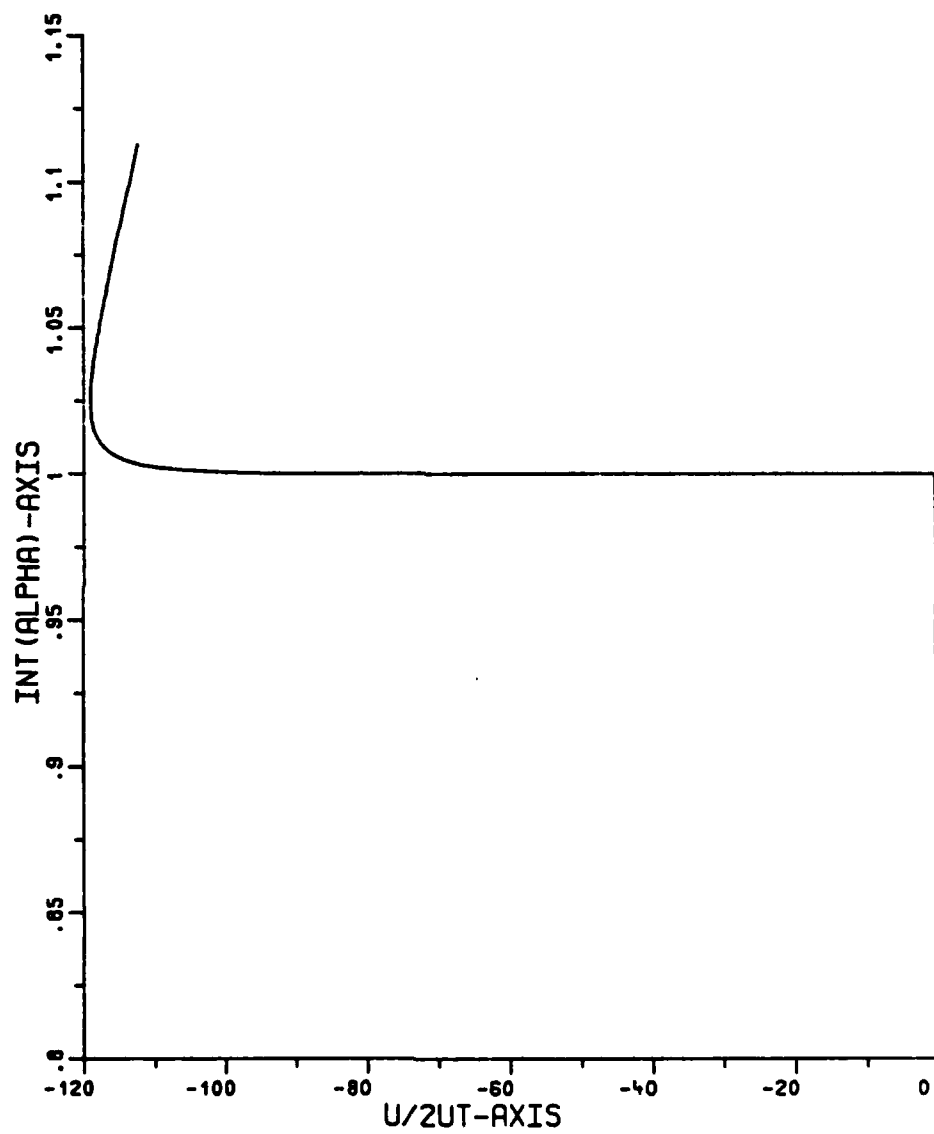


Figure 8



# REFERENCES

1. J. T. Schwartz (1969) 'Nonlinear Functional Analysis', Gordon and Breach Science Publishers.
2. C. Den Heizer and W. C. Rheinboldt (1981) 'On Steplength Algorithms for a Class of Continuation Methods', SIAM J. Numer. Anal., Vol. 18, No. 5, pp. 925-948.
3. H. B. Keller (1975) 'Approximation Methods for Nonlinear Problems with Application to Two-Point-Boundary-Value-Problems', Math. Comp., Vol. 29, pp. 464-474.
4. H. B. Keller (1977) 'Numerical Solution of Bifurcation and Nonlinear Eigenvalue Problems' in 'Applications of Bifurcation Theory', P. H. Rabinowitz, ed., Academic Press, NY.
5. P. A. Markowich (1983a) 'A Singular Perturbation Analysis of the Fundamental Semiconductor Device Equations', submitted to SIAM J. Appl. Math.
6. P. A. Markowich (1983b) 'A Nonlinear Eigenvalue Problem Modelling the Avalanche Effect in Semiconductor Diodes' to appear as MRC Technical Summary Report.
7. P. A. Markowich, C. A. Ringhofer, S. Selberherr and M. Lentini (1983b) 'A Singular Perturbation Approach for the Analysis of the Fundamental Semiconductor Equations' to appear in IEEE J. of Electronic Devices.
8. M. Mock (1983) 'Analysis of Mathematical Models of Semiconductor Devices', Boole Press, Dublin.
9. S. M. Sze (1981) 'Physics of Semiconductor Devices', Second Edition, Wiley Interscience.
10. W. V. Van Roosbroeck (1950) 'Theory of Flow of Electrons and Holes in Germanium and Other Semiconductors', Bell. Syst. Techn. J., Vol. 29, pp. 560-607.

PAM:CAR:AS:scr

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER 2605	2. GOVT ACCESSION NO. A2A137 919	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) COMPUTATION OF CURRENT-VOLTAGE-CHARACTERISTICS IN A SEMICONDUCTOR DEVICE USING ARC-LENGTH CONTINUATION		5. TYPE OF REPORT & PERIOD COVERED Summary Report - no specific reporting period
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Peter A. Markowich, Christian A. Ringhofer, and Alois Steindl		8. CONTRACT OR GRANT NUMBER(s) DAAG29-80-C-0041
9. PERFORMING ORGANIZATION NAME AND ADDRESS Mathematics Research Center, University of 610 Walnut Street Wisconsin Madison, Wisconsin 53706		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Work Unit Number 3 - Numerical Analysis & Scientific Computing
11. CONTROLLING OFFICE NAME AND ADDRESS U. S. Army Research Office P. O. Box 12211 Research Triangle Park, North Carolina 27709		12. REPORT DATE December 1983
		13. NUMBER OF PAGES 20
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Semiconductor devices Characteristics Continuation Newton's method		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This paper is concerned with the computation of semiconductor device current-voltage characteristics. We describe an algorithm which allows the computation of characteristics by continuation in a parameter which approximates the arclength of the characteristic. The use of this parameterization allows the characteristic to continue beyond snap-back-voltages, while continuation in the voltage fails past snap-back-voltages. We discuss the implementation of the parameterization and give a numerical example.		

END

FILMED

3-84

DTIC